

CFD Simulation of Thermodynamic and Temperature Effects on Spontaneous Combustion of Coal Stockpiles and Dumps:

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SUMMARY

In this work the development of a numerical model capable of identifying suitable conditions responsible for spontaneous combustion of coal storage piles and carbonaceous waste dumps are presented. The developed model captured the mass, momentum and energy conservation equations through the porous media. Combustion processes under consideration included physical absorption and desorption of atmospheric species in the coal matrix, formation of coal-oxygen complexes and oxygenated carbon species through chemisorption as well as the formation of both CO₂ and CO through coal oxygenation. The aim of this model was to predict the influence of parameters such as buoyancy driven flows, temperature, storage pile porosity and permeability distributions as well as storage pile geometrical dimensions on combustion characteristics of carbonaceous materials.

Possible analysis of such a model is constructed from the basis of a volume averaged methodology instead of deriving governing equations on a pore scale since this has proven to be the best options both from the time and physical dimensions perspectives. In all the cases strong non-linear interactions between the mass, momentum, and energy balance equations complicated the solution attainment through numerical integration of stiff partial differential equations (PDE's). The simulation results obtained from the two-dimensional model provided useful information in characterising the thermal-flow and combustion properties of coal stockpiles and carbonaceous materials and as such proved to be beneficial in assessing the stability of the stockpiles and quantifying the amount of CO₂ emitted during combustion. The qualitative correctness of the model was validated by comparing the predicted results with other available numerical data obtained from the literature. Good correlations between the predicted and numerical results were obtained

Key Words: Spontaneous Combustion, Coal Stockpiles, Carbonaceous Waste Dumps, Stiff PDE's, CFD Modelling, Volume Averaged Methodology and Adsorption, Desorption and Chemisorptions.

1. INTRODUCTION

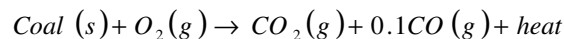
Spontaneous combustion of coal stockpiles and carbonaceous material has long been recognized as both a health and safety hazard by many researchers. This is due to coal and carbonaceous waste dumps being combustible materials when exposed to conducive atmospheric conditions. Given the right amounts of coal, oxygen, temperature and moisture contents, coal will spontaneously self-ignite and thus poses serious health, safety and environmental damages by producing greenhouse gas emissions such as CO₂ and CO and as such needs to be prevented if not eliminated.

The challenge of preventing spontaneous combustion of coal fires requires that mathematical models be constructed in order to improve the understanding of physical phenomenon influencing spontaneous combustion. Some such physical phenomenon includes buoyancy driven flows, temperature as well as thermodynamics effects and porosity distributions of the coal stockpiles. Previous research modelling studies were mainly concerned with investigating burning coal stockpiles without paying much attention of formulating up to date cost effective models capable of preventing or containing the problem. It is therefore believed, that the development of a detail numerical model capable of providing better insight to the problem of spontaneous combustion as well as enabling the formulation of improved preventative measures in this study will be necessary in limiting the damages existing fires causes to the environment.

2. MAIN BODY

2.1 Process description

According to Smith et al (1991) as quoted by Yuan and Smith (2009), the formation of CO₂ and CO from the oxidation of coal is represent by the following exothermic chemical reaction equation:



The formation of CO₂ and CO involves a series of complex processes of physical and desorption of atmospheric species in the coal matrix, formation of coal-oxygenated complexes and carbon species via chemisorptions and formation of gaseous CO₂ and CO products via coal oxidation. As oxygen enriched cool air flow through the porous stockpiles side boundaries via diffusion and convection, coal oxidation reaction then occurs within this homogenous porous medium and as such heated resultant combustion gases then exit through the top of the medium as demonstrated in **Figure 1** below:

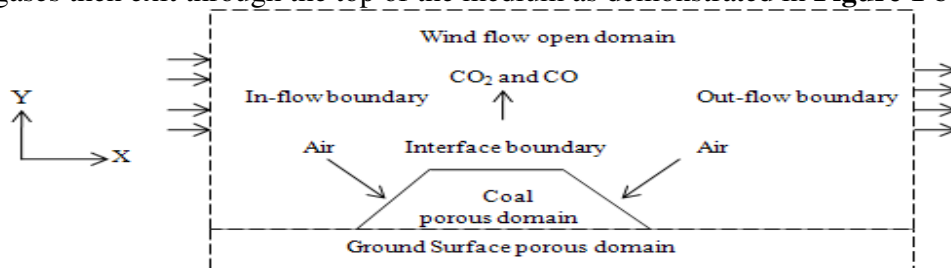


Figure 1: Schematic representation of the computational flow domain

2.2 Methodology

In establishing the dynamic behaviour of the spontaneous heating in coal stockpiles, the following volume-averaged-sets of two dimensional time dependent, strongly coupled nonlinear partial differential equations were employed together with the following additional auxiliary equations.

Air-mixture mass conservation equation in the gas phase was modeled by the following continuity equation:

$$\frac{\partial(\varepsilon \langle \rho_g \rangle^g)}{\partial t} + \frac{\partial}{\partial x_j}(\varepsilon \langle \rho_g \rangle^g \langle u_j \rangle^g) = \langle S_g \rangle^g$$

Momentum conservation equation in the gas phase was modeled by the following momentum transfer equation:

$$\begin{aligned} \frac{\partial}{\partial t}(\varepsilon \langle \rho_g \rangle^g \langle u_k \rangle^g) + \frac{\partial}{\partial x_j}(\varepsilon \langle \rho_g \rangle^g \langle u_j \rangle^g \langle u_k \rangle^g) + \varepsilon \frac{\partial \langle p \rangle^g}{\partial x_k} - \\ \frac{\partial}{\partial x_j} \left(\langle \mu_g \rangle^g \frac{\partial}{\partial x_j} \langle u_j \rangle^g \right) - \varepsilon \langle \rho_g \rangle^g \langle g_k \rangle^g - B_k = S_m \end{aligned}$$

Energy conservation equation for the solid phase was modeled by the following heat transfer equation:

$$\begin{aligned} \frac{\partial}{\partial t}((1 - \varepsilon) \langle \rho_s \rangle^s \langle c_{ps} \rangle \langle T_s \rangle^s) - \frac{\partial}{\partial x_j} \left(k_{eff} \frac{\partial \langle T_s \rangle^s}{\partial x_j} \right) + \\ \frac{6(1 - \varepsilon) h_{gs} (\langle T_s \rangle^s - \langle T_g \rangle^g)}{d_p} = S_o + S_{ec} \end{aligned}$$

The porosity of the coal dump was calculated from Yuan and Smith, (2009):

$$\varepsilon = 1 - \frac{\rho_b}{\rho_p}$$

The Arrhenius rate of oxidation was calculated from Yuan and Smith, (2009)

$$Q = AC \exp(-E/RT)$$

3 RESULTS AND DISCUSSION

The thermodynamic Gibbs free energy values depicted in **Table 1** were calculated with the aim of predicting the feasibility of various reactions mechanisms to be model. As can be seen, favourable conditions for spontaneous reactions were observed for various reaction temperatures.

3.1 Thermodynamic Reaction Feasibility Prediction

Reaction Equations	$\Delta G_{f25^\circ C}^0$ (kJ)	$\Delta G_{f150^\circ C}^0$ (kJ)	$\Delta G_{f230^\circ C}^0$ (kJ)
$CO(g) + H_2O(g) \xrightarrow{k1} H_2(g) + CO_2(g)$	-53.580	-58.942	-63.142
$C(s) + 2H_2(g) \xrightarrow{k2} CH_4(g)$	-50.717	-40.600	-32.506
$CO(g) + 3H_2(g) \xrightarrow{k3} CH_4(g) + H_2O(g)$	-142.120	-115.290	-93.820
$CO_2(g) + C(s) \xrightarrow{k4} 2CO(g)$	-120.057	-98.087	-80.511

Table 1: Thermodynamic Gibbs free energy calculated values for various chemical reaction equations at different temperature ranges.

3.2 Temperature distribution around the coal stockpile

The rate of change of temperature inside and around the coal stockpiles is shown in **Figure 2**. As expected, temperature increased with increases in computational time as depicted. These results are reasonable since minimal increases in temperature attained on the LHS of **Figure 2** is associated with natural convection were as maximum temperature increases attained on the RHS of **Figure 2** is associated with heat generated by oxidation reaction of the carbonaceous material.

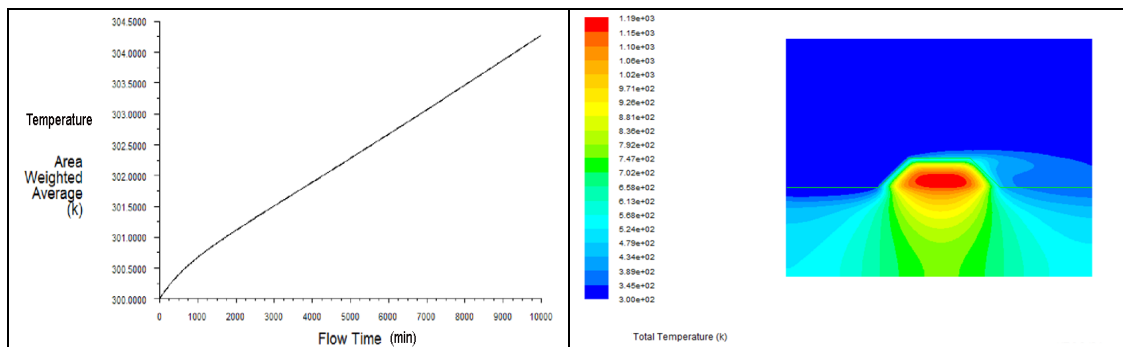


Figure 2: Temporal variation of temperature in the coal dump (LHS) and its associated temperature distributions over the computational flow domain computed at a porosity of 0.3 (RHS).

4. CONCLUSIONS

The overall observation from thermodynamic Gibbs free energy calculations indicated that the reactions are favourable, spontaneous and exergonic and therefore becomes more spontaneous with increases in temperature for all reactions except for the gasification reaction. Moreover, the simulated results obtained from the model were useful information that enabled the tracking of the combustion process from the insufficient temperature rise provided by natural convection leading to spontaneous combustion taking place under high oxidation reaction temperatures.

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